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A NEW VARIATIONAL METHOD FOR INITIAL VALUE PROBLEMS, USING PIECEWISE HERMITE POLYNOMIAL SPLINE FUNCTIONS

C. N. Shen
Julian J. Wu

August 1981

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
LARGE CALIBER WEAPON SYSTEMS LABORATORY
BENÉT WEAPONS LABORATORY
WATERVLIET, N. Y. 12189

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A variational principle for a functional can be found which satisfies both the original system and its adjoint system. The variations of this functional give no boundary terms if the bilinear concomitant of the systems vanishes. For a second order time-varying initial value problem, one can adjust the boundary conditions of the adjoint system in terms of the boundary conditions of the original system so that the bilinear concomitant is identically zero.
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20. ABSTRACT (Cont'd)

An expression for the variation of the functional is derived which contains only the terms involving the variations of the adjoint variable and its derivative, but no variation of its second derivative. The variations of the adjoint variable and its derivative are found to be zeroes at the final conditions, just as the variations of the original variable and its derivative are zero at the starting (initial) conditions. This implies that we are able to solve the problem in one direction without worrying about the conditions at the other end as the initial value problem should be. The algorithm is much more simplified than in the past. An example is given to show the procedures of this new variational method.

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INTRODUCTION

Variational principles apply mostly to boundary problems where eigenvalues are sought. It is seldom used for initial value problems alone where the far end conditions are neither known nor specified. If we use discrete methods to solve an initial value problem, such as finite difference method, only the initial conditions should be given. In the same way, if we employ variational method with spline functions, we should not be concerned with the far end conditions. This paper gives a procedure to find a recursive solution of an initial value problem by variational methods using the cubic hermite polynomial spline functions.

Let us consider a dynamical system governed by the following equation:

$$L(t)y_a(t) = -Q(t) \tag{1}$$

with appropriate boundary conditions. In the above equation L is a linear operator, y_a is the dependent variable, Q is a forcing function, and t is the independent variable.

Some integral property in the form of a linear functional of the variable,[1] such as the inner product of an adjoint forcing function $\bar{Q}$ and the solution of Eq. (1) can be used for estimation.

$$G[y_a] = \int_{t_o}^{t_b} \bar{Q}y_a dt \tag{2}$$

[1]W. M. Stacy, Jr., "Variational Methods in Nuclear Reactor Physics," Academic Press, 1974, p. 7.

The estimate y which differs from the solution y_a of Eq. (1) by an increment δy can be written as

$$\delta y = y - y_a \tag{3}$$

Then the estimate y becomes

$$G[y] = \int_{t_o}^{t_b} \bar{Q}y dt = \int_{t_o}^{t_b} \bar{Q}y_a dt + \int_{t_o}^{t_b} \bar{Q}\delta y dt$$

$$= G[y_a] + \int_{t_o}^{t_b} \bar{Q}\delta y dt \tag{4}$$

which is in error to first order in δy and $\bar{Q}$.

THE VARIATION PRINCIPLE

A more accurate estimate can be made by constructing a variational principle[1] for Eq. (2). By using the adjoint variable $\bar{y}$ as a Lagrange multiplier for Eq. (1) added to $G[y]$ we have

$$J[y,\bar{y}] = G[y] + \int_{t_o}^{t_b} \bar{y}\,(Q+Ly)dt$$

$$= \int_{t_o}^{t_b} \bar{Q}y dt + \int_{t_o}^{t_b} \bar{y}Q dt + \int_{t_o}^{t_b} \bar{y}Ly dt \tag{5}$$

In order that J be a variational principle for G the following requirements must be satisfied.

(a) J is stationary about the function y_s which satisfies the relation in Eq. (1).

$$L(t)y_s = -Q(t) \tag{6}$$

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[1] W. M. Stacy, Jr., "Variational Methods in Nuclear Reactor Physics," Academic Press, 1974, p. 7.

(b) The stationary value of J deduced from Eqs. (2) through (5) is

$$J[\bar{y},y] = G[y_s] + G[y_a] \tag{7}$$

Consider first the stationarity of J by taking the variation

$$\delta J = \delta\left\{\int_{t_o}^{t_b} \bar{Q}y\,dt + \int_{t_o}^{t_b} \bar{y}Q\,dt + \int_{t_o}^{t_b} \bar{y}Ly\,dt\right\}$$

$$\delta J = \int_{t_o}^{t_b} \delta\bar{y}(Ly+Q)dt + \int_{t_o}^{t_b} [\bar{Q}\delta y + \bar{y}L\delta y]dt \tag{8}$$

We will make an effort later to impose certain conditions in order that the following equality holds:

$$\int_{t_o}^{t_b} \bar{y}L\delta y\,dt = \int_{t_o}^{t_b} \delta y\overline{Ly}\,dt \tag{9}$$

where $\bar{L}(t)$ is an adjoint operator.

By combining Eqs. (8) and (9) one obtains

$$\delta J = \int_{t_o}^{t_b} \delta\bar{y}(Ly+Q)dt + \int_{t_o}^{t_b} \delta y[\overline{Ly} + \bar{Q}]dt = 0 \tag{10}$$

Since the variations $\delta\bar{y}$ and δy are arbitrary it leads to the requirement that the stationary values y_s and $\bar{y}_s$ must satisfy

$$Ly_s = -Q \tag{11}$$

$$\overline{Ly}s = -\bar{Q} \quad . \tag{12}$$

Since Eq. (11) is the same as Eq. (6), therefore J is stationary about the function y_s. Equation (12) is the adjoint equation in terms of the adjoint operator $\bar{L}$, the adjoint variable $\bar{y}$, and the adjoint forcing function $\bar{Q}$.

Using the relation in Eq. (11) for the stationary value of J from Eq. (5) we have

$$J[\bar{y}_s\ y_s] = \int_{t_o}^{t_b} Q\bar{y}_s dt + \int_{t_o}^{t_b} \bar{y}_s(Q+Ly_s)dt = G[y_s] \tag{13}$$

Since J is stationary and $\delta J \rightarrow 0$ then

$$G[y_s] \rightarrow G[y_a] \tag{14}$$

which is the requirement given in Eq. (7).

It is noted that Eq. (10) contains no boundary terms to be satisfied. This bears an important point in the future discussion of the initial value problems.

BILINEAR CONCOMITANT

The assumed equality in Eq. (9) is discussed here by considering the following bilinear concomitant:[1]

$$D = \int_{t_o}^{t_b} \bar{y}Lydt - \int_{t_o}^{t_b} y\bar{L}\bar{y}dt \tag{15}$$

The above expression can also be written in terms of boundary conditions at $t = t_o$ and $t = t_b$. It is assumed that these boundary conditions are assigned in such a way that the above bilinear concomitant is identically zero, i.e.,

$$D \equiv 0 \tag{16}$$

[1]W. M. Stacy, Jr., "Variational Methods in Nuclear Reactor Physics," Academic Press, 1974, p. 7.

Then the first variations of D also vanish.

$$\delta D = \delta D(\delta\bar{y}) + \delta D(\delta y) = 0 \tag{17}$$

Since $\delta\bar{y}$ and δy are independent of each other, then

$$\delta D(\delta\bar{y}) = \int_{t_o}^{t_b} \delta\bar{y}Ly\,dt - \int_{t_o}^{t_b} y\bar{L}\delta\bar{y}\,dt = 0 \tag{18}$$

and

$$\delta D(\delta y) = \int_{t_o}^{t_b} \bar{y}L\delta y\,dt - \int_{t_o}^{t_b} \delta y\bar{L}\bar{y}\,dt = 0 \tag{19}$$

Equation (19) is identical to Eq. (9), which is the assumed equality previously. This implies that if Eq. (16) is true then Eq. (9) or (19) is automatically true.

INTEGRAL OF BILINEAR EXPRESSION

The integral of a function is given as

$$I = \int_{t_o}^{t_b} \psi(y\bar{y})\,dt \tag{20}$$

where $\psi(y\bar{y})$ is an arbitrary bilinear expression[2] in the form

$$\psi(y\bar{y}) = \alpha y'\bar{y}' + \beta y'\bar{y} + \gamma y\bar{y}' + \varepsilon y\bar{y} \tag{21}$$

The prime (') in the above expression denotes (d/dt).

Equation (20) can be integrated by parts. Two different forms of integration and end conditions may be obtained as follows.

$$I = -\int_{t_o}^{t_b} \bar{y}Ly\,dt + (\alpha y'+\gamma y)\bar{y}\Big|_{t_o}^{t_b} \tag{22}$$

[2] R. Courant and D. Hilbert, "Methods of Mathematical Physics, Vol. I," Interscience Publishers Inc., 1953, p. 278.

or

$$I = -\int_{t_o}^{t_b} y\bar{L}\bar{y}dt + (\alpha\bar{y}'+\beta\bar{y})y\Big|_{t_o}^{t_b} \tag{23}$$

where the differential expressions are

$$Ly = (\alpha y')' - \beta y' + (\alpha y)' - \varepsilon y \tag{24}$$

$$\bar{L}\bar{y} = (\alpha\bar{y}')' + (\beta\bar{y})' - \gamma\bar{y}' - \varepsilon\bar{y} \tag{25}$$

The bilinear concomitant given in Eq. (15) can now be expressed in terms of the function values and their derivatives at the end points by equating Eqs. (22) and (23).

$$D = [\alpha(y'\bar{y}-\bar{y}'y) - (\gamma-\beta)y\bar{y}]\Big|_{t_o}^{t_b} \tag{26}$$

END CONDITIONS FOR THE ADJOINT SYSTEM

In order to satisfy the expression $D \equiv 0$ in Eqs. (15) and (16) the end terms in Eq. (26) must vanish. Thus it requires

$$\alpha_b(y_b'\bar{y}_b-\bar{y}_b'y_b) - \alpha_o(y_o'\bar{y}_o-\bar{y}_o'y_o) - (\gamma_b-\beta_b)y_b\bar{y}_b + (\gamma_o-\beta_o)y_o\bar{y}_o \equiv 0 \tag{27}$$

Equation (27) can be satisfied identically if the end conditions of the adjoint system are proportional to the end conditions of the original system as follows:

$$\bar{y}_b = (\gamma_o-\beta_o)ky_o \tag{28a}$$

$$\bar{y}_o = (\gamma_b-\beta_b)ky_b \tag{28b}$$

$$\bar{y}_b' = -\alpha_b^{-1}\alpha_o(\gamma_b-\beta_b)ky_o' \tag{28c}$$

$$\bar{y}_b' = -\alpha_o^{-1}\alpha_b(\gamma_o-\beta_o)ky_b' \tag{28d}$$

where k is a constant.

The above expressions give the required end conditions for the adjoint system in terms of that of the original system. Thus from Eqs. (15) and (16):

$$D = \int_{t_o}^{t_b} \bar{y}Ly\,dt - \int_{t_o}^{t_b} \overline{yL}y\,dt \equiv 0 \qquad (29)$$

To summarize, if one can make the end conditions of the adjoint system satisfy the relationship in Eq. (28), the bilinear concomitent D vanishes. The variation in Eq. (10) is then valid.

It is also noted that the variation in Eq. (10) has no far end terms which simplify the computation. This is because the far end terms may cause certain difficulties in many computational schemes on a number of variational methods.

THE FIRST VARIATION

Since the variations $\delta\bar{y}$ and δy are independent to each other, we take the first half of Eq. (10) as

$$\delta J(\delta\bar{y}) = \int_{t_o}^{t_b} \delta\bar{y}Ly\,dt + \int_{t_o}^{t_b} \delta\bar{y}Q\,dt = 0 \qquad (30)$$

Equation (30) is not in a ready form for estimation. We prefer to use δI which can be obtained from the bilinear expression I given in Eqs. (20) and (21). Let

$$\delta I = \delta I(\delta\bar{y}) + \delta I(\delta y) \qquad (31)$$

The first part of the above expression can be derived from Eqs. (20) and (21) as

$$\delta I(\delta\bar{y}) = \int_{t_o}^{t_b} [(\alpha y'+\gamma y)\delta\bar{y}' + (\beta y'+\epsilon y)\delta\bar{y}]dt \qquad (32)$$

Integrating by parts one obtains

$$\delta I(\delta\bar{y}) = (\alpha y'+\gamma y)\delta\bar{y}\Big|_{t_o}^{t_b} - \int_{t_o}^{t_b} \delta\bar{y}[(\alpha y'+\gamma y)' - (\beta y'+\epsilon y)]dt \tag{33}$$

It is recognized that the integrand in the last term of the above formulae is Ly. Solving for the last term we have

$$\int_{t_o}^{t_b} \delta\bar{y}Lydt = (\alpha y'+\gamma y)\delta\bar{y}\Big|_{t_o}^{t_b} - \delta I(\delta\bar{y}) \tag{34}$$

Substituting Eq. (32) into (34) and then Eq. (34) into (30) one obtains

$$\begin{aligned} \delta J(\delta\bar{y}) = {} & (\alpha_b y_b'+\gamma_b y_o)\delta\bar{y}_b - (\alpha_o y_o'+\gamma_o y_o)\delta\bar{y}_o \\ & - \int_{t_o}^{t_b} [(\alpha y'+\gamma y)\delta\bar{y}' + (\beta y'+\epsilon y)\delta\bar{y}]dt \\ & + \int_{t_o}^{t_b} \delta\bar{y}Qdt = 0 \end{aligned} \tag{35}$$

The above equation contains only $\delta\bar{y}$ and $\delta\bar{y}'$ and none of the variation of the higher derivative such as $\delta\bar{y}''$ for a second order system. The dependent variable also contains only y and y' and none of the higher derivative such as y'' for a second order system.

ADJOINT VARIABLE FAR END VALUE FOR INITIAL VALUE PROBLEMS

For a second order system the initial values of the function and its first derivative are given, i.e., y_o and y_o' are known in Eq. (28). The far end values for the adjoint system $\bar{y}_b$ and $\bar{y}_b'$ are found from Eqs. (28a) and (28c). Since the variation of a constant is zero, then

$$\delta y_o = \delta y_o' = 0 \tag{36}$$

and

$$\delta\bar{y}_b = \delta\bar{y}_b' = 0 \tag{37}$$

The conclusion $\delta\bar{y}_b = 0$ in Eq. (37) is important in that the first term at the right side of Eq. (35) vanishes. Thus the coefficient of $\delta\bar{y}_b$ is <u>not</u> necessarily zero. This implies that the function y_b and its derivative y_b' at the far end are not related as such. By not using any local boundary conditions at the far end, the computation can start at the near end and carry on in one direction.

Thus Eq. (35) is simplified to

$$\delta J(\delta\bar{y}) = -(\gamma_o y_o + \alpha_o y_o')\delta\bar{y}_o + \int_{t_o}^{t_b} \delta\bar{y} Q dt$$

$$-\int_{t_o}^{t_b} [(\varepsilon y + \beta y')\delta\bar{y} + (\gamma y + \alpha y')\delta\bar{y}']dt \tag{38}$$

It is noted that the above equation does not have boundary terms to be satisfied at the far end at time t_b. This is consistent with the notion of "initial value problem" physically.

TRANSFORMATION OF COORDINATES

The integral sign in Eq. (38) can be converted into a summation sign if discrete intervals for integration are used. Since the analysis is an initial value problem, without losing any generality we may let

$$t_o = 0 \quad \text{and} \quad t_b = 1 \quad , \tag{39}$$

that is the independent variable is within the interval

$$0 < t < 1 \tag{40}$$

Equation (38) can be discretized by letting

$$\xi = Kt - m + 1 \tag{41}$$

$$0 < \xi < 1, \quad 0 < t < 1, \quad m = 1,2,\ldots K \tag{42}$$

where K is the number of intervals.

Thus

$$d\xi = Kdt \qquad dt = K^{-1}d\xi \tag{43}$$

The differential relationship is

$$\frac{dy}{dt} = K\frac{dy}{d\xi} \tag{44}$$

or

$$y' = K\dot{y} \tag{45}$$

where

$$(\dot{\ }) = \frac{d}{d\xi}(\ ) \tag{46}$$

Then Eq. (38) becomes

$\delta J(\delta y) = 0$

$$= -(\gamma_o y_o + \alpha_o K\dot{y}_o)\delta\bar{y}_o + \sum_{m=1}^{K}\int_0^1 \delta\bar{y}^{(m)}QK^{-1}d\xi$$

$$- \sum_{m=1}^{K}\int_0^1 [(\epsilon y^{(m)} + \beta K\dot{y}^{(m)})\delta\bar{y}^{(m)} + \{(\gamma y^{(m)} + \alpha K\dot{y}^{(m)}\}K\delta\dot{\bar{y}}^{(m)}]K^{-1}d\xi \tag{47}$$

PIECEWISE SPLINE FUNCTIONS

We may express the variables $y^{(m)}$ and $\bar{y}^{(m)}(\xi)$ in terms of piecewise spline function $a^T(\xi)$ and the node point functions $Y^{(m)}$ and $\bar{Y}^{(m)}$ as follows.

$$y^{(m)}(\xi) = a^T(\xi)\ Y^{(m)} \qquad \delta y^{(m)} = [\delta Y^{(m)}]^T a(\xi) \tag{48}$$

$$\dot{y}^{(m)}(\xi) = \dot{a}^T(\xi)\ Y^{(m)} \qquad \delta\dot{y}^{(m)} = [\delta Y^{(m)}]^T \dot{a}(\xi) \tag{49}$$

$$\bar{y}^{(m)}(\xi) = a^T(\xi)\bar{Y}^{(m)} \qquad \delta\bar{y}^{(m)} = [\delta\bar{Y}^{(m)}]^T a(\xi) \tag{50}$$

$$\dot{\bar{y}}^{(m)}(\xi) = \dot{a}^T(\xi)\bar{Y}^{(m)} \qquad \delta\dot{\bar{y}}^{(m)} = [\delta\bar{Y}^{(m)}]^T \dot{a}(\xi) \tag{51}$$

$$m = 1,2,\ldots K$$

$$y_o \overset{\Delta}{=} a^T(1)Y^{(o)} \tag{52}$$

$$\dot{y}_o \overset{\Delta}{=} \dot{a}^T(1)Y^{(o)} \tag{53}$$

$$\delta\bar{y}_o \overset{\Delta}{=} \delta\bar{Y}^{(o)}a(1) \tag{54}$$

If Eqs. (48) through (54) are substituted into Eq. (47) one obtains

$$0 = -[\delta\bar{Y}^{(o)}]^T a(1)[\gamma_o a^T(1) + \alpha_o K\dot{a}^T(1)]Y^{(o)}$$
$$+ \sum_{m=1}^{K} [\delta\bar{Y}^{(m)}]^T K^{-1} \int_0^1 a(\xi)Qd\xi$$
$$- \sum_{m=1}^{K} [\delta Y^{(m)}]^T \int_0^1 a(\xi)[\epsilon K^{-1}a^T(\xi) + \beta\dot{a}^T(\xi)]d\xi \; Y^{(m)}$$
$$- \sum_{m=1}^{K} [\delta\bar{Y}^{(m)}]^T \int_0^1 \dot{a}(\xi)[\gamma a^T(\xi) + \alpha K\dot{a}^T(\xi)]d\xi \; Y^{(m)} \tag{55}$$

This simplifies to

$$0 = -[\delta\bar{Y}^{(o)}]^T a(1)[\gamma_o a^T(1) + \alpha_o K\dot{a}^T(1)]Y^{(o)}$$
$$+ \sum_{m=1}^{K} [\delta\bar{Y}^{(m)}]^T q^{(m)} - \sum_{m=1}^{K} [\delta\bar{Y}^{(m)}]^T \, p^{(m)} \; Y^{(m)} \tag{56}$$

where

$$q^{(m)} = K^{-1} \int_0^1 a(\xi)Q(\xi)d\xi$$
$$= [q_1^{(m)}, q_2^{(m)}, q_3^{(m)}, q_4^{(m)}]^T \tag{57}$$

and

$$p^{(m)} = \int_0^1 \{a(\xi)[\epsilon^{(m)}K^{-1}a^T(\xi) + \beta^{(m)}\dot{a}^T(\xi)] + \dot{a}(\xi)[\gamma^{(m)}a^T(\xi) + \alpha^{(m)}K\dot{a}^T(\xi)]\}d\xi$$
$$= \epsilon^{(m)}K^{-1}B + \beta^{(m)}C + \gamma^{(m)}D + \alpha^{(m)}KE \tag{58}$$

or

$$[p_{ij}^{(m)}] = \epsilon^{(m)}K^{-1}[b_{ij}] + \beta^{(m)}[c_{ij}] + \gamma^{(m)}[d_{ij}] + \alpha^{(m)}K[e_{ij}] \tag{59}$$

where

$$B = [b_{ij}] = \int_0^1 a(\xi)a^T(\xi)d\xi \tag{60}$$

$$C = [c_{ij}] = \int_0^1 a(\xi)\dot{a}^T(\xi)d\xi \tag{61}$$

$$D = [d_{ij}] = \int_0^1 \dot{a}(\xi)a^T(\xi)d\xi \tag{62}$$

$$E = [e_{ij}] = \int_0^1 \dot{a}(\xi)\dot{a}^T(\xi)d\xi \tag{63}$$

CUBIC HERMITE POLYNOMIAL SPLINE

The cubic Hermite polynomial spline is continuous in the functional values and its first derivatives across the nodes. Since we have no second derivatives for $a(\xi)$ in Eqs. (58) to (63), no higher order spline is necessary for this problem.

The cubic Hermite polynomial gives

$$a(\xi) = \begin{bmatrix} a_1(\xi) & = & 1-3\xi^2+2\xi^3 \\ a_2(\xi) & = & \xi-2\xi^2+\xi^3 \\ a_3(\xi) & = & 3\xi^2-2\xi^3 \\ a_4(\xi) & = & -\xi^2+\xi^3 \end{bmatrix} \tag{64}$$

whose derivatives are

$$\dot{a}(\xi) = \begin{bmatrix} \dot{a}_1(\xi) & = & -6\xi+6\xi^2 \\ \dot{a}_2(\xi) & = & 1-4\xi+3\xi^2 \\ \dot{a}_3(\xi) & = & 6\xi-6\xi^2 \\ \dot{a}_4(\xi) & = & -2\xi+3\xi^2 \end{bmatrix} \tag{65}$$

It is obvious from the above equations that the node point values are

$$a(0) = [a_1(0)\ a_2(0)\ a_3(0)\ a_4(0)]^T$$

$$= [\ 1 \quad 0 \quad 0 \quad 0\ ]^T \tag{66a}$$

$$\dot{a}(0) = [\dot{a}_1(0)\ \dot{a}_2(0)\ \dot{a}_3(0)\ \dot{a}_4(0)]^T$$

$$= [\ 0 \quad 1 \quad 0 \quad 0\ ]^T \tag{66b}$$

$$a(1) = [a_1(1)\ a_2(1)\ a_3(1)\ a_4(1)]^T$$

$$= [\ 0 \quad 0 \quad 1 \quad 0\ ]^T \tag{66c}$$

$$\dot{a}(1) = [\dot{a}_1(1)\ \dot{a}_2(1)\ \dot{a}_3(1)\ \dot{a}_4(1)]^T$$

$$= [\ 0 \quad 0 \quad 0 \quad 1\ ]^T \tag{66d}$$

We wish to form a vector whose components are taken from the function and its derivative at the left node and then the same at the right node. From Eqs. (48), (49), and (66) we have

$$\begin{bmatrix} y^{(m)}(0) \\ \dot{y}^{(m)}(0) \\ y^{(m)}(1) \\ \dot{y}^{(m)}(1) \end{bmatrix} = \begin{bmatrix} a^T(0)Y^{(m)} \\ \dot{a}^T(0)Y^{(m)} \\ a^T(1)Y^{(m)} \\ \dot{a}^T(1)Y^{(m)} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} Y^{(m)} = Y^{(m)} \tag{67}$$

If we define

$$Y^{(m)} = [Y_1^{(m)}\ Y_2^{(m)}\ Y_3^{(m)}\ Y_4^{(m)}]^T \tag{68}$$

Then

$$Y_1^{(m)} = y^{(m)}(0) \tag{69a}$$

$$Y_2^{(m)} = \dot{y}^{(m)}(0) \tag{69b}$$

$$Y_3^{(m)} = y^{(m)}(1) \tag{69c}$$

$$Y_4^{(m)} = \dot{y}^{(m)}(1) \tag{69d}$$

The above implies that the same node point has been represented by two notations as follows

$$y^{(m+1)}(0) = y^{(m)}(1) \tag{70a}$$

$$\dot{y}^{(m+1)}(0) = \dot{y}^{(m)}(1) \tag{70b}$$

By expanding Eq. (68) for different m one obtains

$$Y^{(0)} = [0\ 0\ Y_3^{(0)}\ Y_4^{(0)}]^T = [0\ 0\ y^{(0)}(1)\ y^{(0)}(1)]^T \tag{71a}$$

$$Y^{(1)} = [Y_1^{(1)}\ Y_2^{(1)}\ Y_3^{(1)}\ Y_4^{(1)}]^T = [y^{(1)}(0)\ \dot{y}^{(1)}(0)\ y^{(1)}(1)\ \dot{y}^{(1)}(1)]^T \tag{71b}$$

$$Y^{(m)} = [Y_1^{(m)}\ Y_2^{(m)}\ Y_3^{(m)}\ Y_4^{(m)}]^T = [y^{(m)}(0)\ \dot{y}^{(m)}(0)\ y^{(m)}(1)\ \dot{y}^{(m)}(1)]^T \tag{71c}$$

$$Y^{(m+1)} = [Y_1^{(m+1)}\ Y_2^{(m+1)}\ Y_3^{(m+1)}\ Y_4^{(m+1)}]^T = [y^{(m+1)}(0)\ \dot{y}^{(m+1)}(0)\ y^{(m+1)}(1)\ \dot{y}^{(m+1)}(1)]^T \tag{71d}$$

Thus we have

$$Y_1^{(m+1)} = Y_3^{(m)} \tag{72a}$$

and

$$Y_2^{(m+1)} = Y_4^{(m)} \tag{72b}$$

for $m = 0,1,2,...K$.

Similar to the above equation one can prove from Eqs. (50) and (51) that the adjoint variations are

$$\delta\bar{Y}_1^{(m+1)} = \delta\bar{Y}_3^{(m)} \tag{73a}$$

and

$$\delta\bar{Y}_2^{(m+1)} = \delta\bar{Y}_4^{(m)} \tag{73b}$$

METHOD OF SOLUTIONS

First we take the last term of Eq. (56) which is

$$R_3 = -\sum_{m=1}^{K} [\delta Y_1^{(m)}\ \delta Y_2^{(m)}\ \delta Y_3^{(m)}\ \delta Y_4^{(m)}][p_{ij}^{(m)}][Y_1^{(m)}\ Y_2^{(m)}\ Y_3^{(m)}\ Y_4^{(m)}]T \tag{74}$$

Using the relationship from Eqs. (72) and (73) gives

$$\begin{aligned}R_3 = -\sum_{m=1}^{K} \{&[p_{11}^{(m)}Y_3^{(m+1)} + p_{12}^{(m)}Y_4^{(m-1)} + p_{13}^{(m)}Y_3^{(m)} + p_{14}^{(m)}Y_4^{(m)}]\delta\bar{Y}_3^{(m-1)}\\ &+ [p_{21}^{(m)}Y_3^{(m-1)} + p_{22}^{(m)}Y_4^{(m-1)} + p_{23}^{(m)}Y_3^{(m)} + p_{24}^{(m)}Y_4^{(m)}]\delta\bar{Y}_4^{(m-1)}\\ &+ [p_{31}^{(m)}Y_3^{(m-1)} + p_{32}^{(m)}Y_4^{(m-1)} + p_{33}^{(m)}Y_3^{(m)} + p_{34}^{(m)}Y_4^{(m)}]\delta\bar{Y}_3^{(m)}\\ &+ [p_{41}^{(m)}Y_3^{(m-1)} + p_{42}^{(m)}Y_4^{(m-1)} + p_{43}^{(m)}Y_3^{(m)} + p_{44}^{(m)}Y_4^{(m)}]\delta\bar{Y}_4^{(m)}\}\end{aligned} \tag{75}$$

$$\begin{aligned}R_3 = &- [p_{11}^{(1)}Y_3^{(0)} + p_{12}^{(1)}Y_4^{(0)} + p_{13}^{(1)}Y_3^{(1)} + p_{14}^{(1)}Y_4^{(1)}]\delta\bar{Y}_3^{(0)}\\ &- [p_{21}^{(1)}Y_3^{(0)} + p_{22}^{(1)}Y_4^{(0)} + p_{23}^{(1)}Y_3^{(1)} + p_{24}^{(1)}Y_4^{(1)}]\delta\bar{Y}_4^{(0)}\\ &-\sum_{m=1}^{K-1} \{[p_{11}^{(m+1)}Y_3^{(m)} + p_{12}^{(m+1)}Y_4^{(m)} + p_{13}^{(m+1)}Y_3^{(m+1)} + p_{14}^{(m+1)}Y_4^{(m+1)}]\\ &+ [p_{31}^{(m)}Y_3^{(m-1)} + p_{32}^{(m)}Y_4^{(m-1)} + p_{33}^{(m)}Y_3^{(m)} + p_{34}^{(m)}Y_4^{(m)}]\}\delta\bar{Y}_3^{(m)}\\ &-\sum_{m=1}^{K-1} \{[p_{21}^{(m+1)}Y_3^{(m)} + p_{22}^{(m+1)}Y_4^{(m)} + p_{23}^{(m+1)}Y_3^{(m+1)} + p_{24}^{(m+1)}Y_4^{(m+1)}]\\ &+ [p_{41}^{(m)}Y_3^{(m-1)} + p_{42}^{(m)}Y_4^{(m-1)} + p_{43}^{(m)}Y_3^{(m)} + p_{44}^{(m)}Y_4^{(m)}]\}\delta\bar{Y}_4^{(m)}\\ &- [p_{31}^{(K)}Y_3^{(K-1)} + p_{32}^{(K)}Y_4^{(K-1)} + p_{33}^{(K)}Y_3^{(K)} + p_{34}^{(K)}Y_4^{(K)}]\delta\bar{Y}_3^{(K)}\\ &- [P_{41}^{(K)}Y_3^{(K-1)} + p_{42}Y_4^{(K-1)} + p_{43}^{(K)}Y_3^{(K)} + p_{44}^{(K)}Y_4^{(K)}]\delta\bar{Y}_4^{(K)}\end{aligned} \tag{76}$$

It is noted here that the variations at the far end are

$$\delta\bar{Y}_3^{(K)} = \delta\bar{y}_b = 0 \tag{77}$$

$$\delta\bar{Y}_4^{(K)} = \delta\bar{y}_b' = 0 \tag{78}$$

by virtue of Eqs. (36) and (37). Thus the last two terms of Eq. (76) drop out.

It is again important to emphasize here that the computation does not contain the condition placed at the far end boundary. The calculation starts with the initial conditions and carries through in one direction.

The second term on the right side of Eq. (56) gives

$$
\begin{aligned}
R_2 &= \sum_{m=1}^{K} [q_1^{(m)}\ q_2^{(m)}\ q_3^{(m)}\ q_4^{(m)}][\delta\bar{Y}_3^{(m-1)}\ \delta\bar{Y}_4^{(m-1)}\ \delta\bar{Y}_3^{(m)}\ \delta\bar{Y}_4^{(m)}]^T \\
&= q_1^{(1)}\delta\bar{Y}_3^{(0)} + q_2^{(1)}\delta\bar{Y}_4^{(0)} \\
&+ \sum_{m=1}^{K-1} [q_1^{(m+1)} + q_3^{(m)}]\delta\bar{Y}_3^{(m)} + \sum_{m=1}^{K-1} [q_2^{(m+1)} + q_4^{(m)}]\delta\bar{Y}_4^{(m)} \\
&+ q_3^{(K)}\delta\bar{Y}_3^{(K)} + q_4^{(K)}\delta\bar{Y}_4^{(K)} \qquad (79)
\end{aligned}
$$

The last two terms drop out again by virtue of Eqs. (77) and (78) .

The quantity $q^{(m)}$ is again expressed as

$$
q_\ell^{(m)} = K^{-1} \int_0^1 a_\ell(\xi)Q^{(m)}(\xi)d\xi \qquad \ell = 1,2,3,4 \qquad (80)
$$

The first term on the right of Eq. (56) is

$$
\begin{aligned}
R_1 &= -[0\ 0\ \delta\bar{Y}_3^{(0)}\ \delta\bar{Y}_4^{(0)}][0\ 0\ 1\ 0]^T\{\gamma_o[0\ 0\ 1\ 0] + \alpha_o K[0\ 0\ 0 1]\}[0\ 0\ Y_3^{(0)} Y_4^{(0)}]^T \\
&= -\delta Y_3^{(0)}\{\gamma_o Y_3^{(0)} + \alpha_o K Y_4^{(0)}\} \qquad (81)
\end{aligned}
$$

Combining all the above results and substituting into Eq. (56) we have

$$
0 = R_1 + R_2 + R_3 \qquad (82)
$$

by virtue of Eqs. (36) and (37). Thus the last two terms of Eq. (76) drop out.

It is again important to emphasize here that the computation does not contain the condition placed at the far end boundary. The calculation starts with the initial conditions and carries through in one direction.

The second term on the right side of Eq. (56) gives

$$R_2 = \sum_{m=1}^{K} [q_1^{(m)}\ q_2^{(m)}\ q_3^{(m)}\ q_4^{(m)}][\delta\bar{Y}_3^{(m-1)}\ \delta\bar{Y}_4^{(m-1)}\ \delta\bar{Y}_3^{(m)}\ \delta\bar{Y}_4^{(m)}]^T$$

$$= q_1^{(1)}\delta\bar{Y}_3^{(0)} + q_2^{(1)}\delta\bar{Y}_4^{(0)}$$

$$+ \sum_{m=1}^{K-1} [q_1^{(m+1)} + q_3^{(m)}]\delta\bar{Y}_3^{(m)} + \sum_{m=1}^{K-1} [q_2^{(m+1)} + q_4^{(m)}]\delta\bar{Y}_4^{(m)}$$

$$+ q_3^{(K)}\delta\bar{Y}_3^{(K)} + q_4^{(K)}\delta\bar{Y}_4^{(K)} \tag{79}$$

The last two terms drop out again by virtue of Eqs. (77) and (78) .

The quantity $q^{(m)}$ is again expressed as

$$q_\ell^{(m)} = K^{-1} \int_0^1 a_\ell(\xi)Q^{(m)}(\xi)d\xi \qquad \ell = 1,2,3,4 \tag{80}$$

The first term on the right of Eq. (56) is

$$R_1 = -[0\ 0\ \delta\bar{Y}_3^{(0)}\ \delta\bar{Y}_4^{(0)}][0\ 0\ 1\ 0]^T\{\gamma_o[0\ 0\ 1\ 0] + \alpha_oK[0\ 0\ 0 1]\}[0\ 0\ Y_3^{(0)}Y_4^{(0)}]^T$$

$$= -\delta Y_3^{(0)}\{\gamma_oY_3^{(0)} + \alpha_oKY_4^{(0)}\} \tag{81}$$

Combining all the above results and substituting into Eq. (56) we have

$$0 = R_1 + R_2 + R_3 \tag{82}$$

$$
\begin{aligned}
0 = & \{-\{\gamma_o Y_3^{(0)} + \alpha_o K Y_4^{(0)}\} \\
& + q_1^{(1)} - [p_{11}^{(1)} Y_3^{(0)} + p_{12}^{(1)} Y_4^{(0)} + p_{13}^{(1)} Y_3^{(1)} + p_{14}^{(1)} Y_4^{(1)}]\} \delta \bar{Y}_3^{(0)} \\
& + \{q_2^{(1)} - [p_{21}^{(1)} Y_3^{(0)} + p_{22}^{(1)} Y_4^{(0)} + p_{23} Y_3^{(1)} + p_{24}^{(1)} Y_4^{(1)}]\} \delta \bar{Y}_4^{(0)} \\
& + \sum_{m=1}^{K-1} \{[q_1^{(m+1)} + q_3^{(m)}] \\
& - [p_{11}^{(m+1)} Y_3^{(m)} + p_{12}^{(m+1)} Y_4^{(m)} + p_{13}^{(m+1)} Y_3^{(m+1)} + p_{14}^{(m+1)} \ Y_4^{(m+1)}] \\
& - [p_{31}^{(m)} Y_3^{(m-1)} + p_{32}^{(m)} Y_4^{(m-1)} + p_{33}^{(m)} Y_3^{(m)} + p_{34}^{(m)} Y_4^{(m)}]\} \delta \bar{Y}_3^{(m)} \\
& + \sum_{m=1}^{K-1} \{q_2^{(m+1)} + q_4^{(m)}] \\
& - [p_{21}^{(m+1)} Y_3^{(m)} + p_{22}^{(m+1)} Y_4^{(m)} + p_{23}^{(m+1)} Y_3^{(m+1)} + p_{24}^{(m+1)} Y_4^{(m+1)}] \\
& - [p_{41}^{(m)} Y_3^{(m-1)} + p_{42}^{(m)} Y_4^{(m-1)} + p_{43}^{(m)} Y_3^{(m)} + p_{44}^{(m)} Y_4^{(m)}]\} \delta \bar{Y}_4^{(m)} \qquad (83)
\end{aligned}
$$

RECURSIVE SOLUTIONS

Since the variations $\delta\bar{Y}_3^{(0)}$, $\delta\bar{Y}_4^{(0)}$, $\delta\bar{Y}_3^{(m)}$, and $\delta\bar{Y}_4^{(m)}$ in Eq. (83) are all arbitrary, the coefficients of all these variations must vanish. We first take the coefficients of the variations $\delta Y_3^{(0)}$ and $\delta Y_4^{(0)}$.

$$
\begin{bmatrix} p_{13}^{(1)} & p_{14}^{(1)} \\ p_{23}^{(1)} & p_{24}^{(1)} \end{bmatrix}
\begin{bmatrix} Y_3^{(1)} \\ Y_4^{(1)} \end{bmatrix}
=
\begin{bmatrix} (-p_{11}^{(1)} - \gamma_o) & (-p_{12}^{(1)} - \alpha_o K) \\ (-p_{21}^{(1)} & (-p_{22}^{(1)} \end{bmatrix}
\begin{bmatrix} Y_3^{(0)} \\ Y_4^{(0)} \end{bmatrix}
+
\begin{bmatrix} q_1^{(1)} \\ q_2^{(1)} \end{bmatrix}
\qquad (84)
$$

It is noted that $Y_3^{(0)}$ and $Y_4^{(0)}$ are the initial conditions of the problem that is from Eq. (67) and (46).

$$
Y_3^{(0)} = y_o \qquad (85)
$$

$$
Y_4^{(0)} = \dot{y}_o = K^{-1} y_o' = K^{-1} \frac{dy}{dt} \qquad (86)
$$

We can solve for $Y_3(1)$ and $Y_4(1)$ in terms of these initial conditions by inverting the two by two matrix in Eq. (84).

$$\begin{bmatrix} Y_3^{(1)} \\ Y_4^{(1)} \end{bmatrix} = \begin{bmatrix} p_{13}^{(1)} & p_{14}^{(1)} \\ p_{23}^{(1)} & p_{24}^{(1)} \end{bmatrix}^{-1} \left\{ \begin{bmatrix} (-p_{11}^{(1)}-\gamma_o) & (-p_{12}-\alpha_o K) \\ (-p_{21}^{(1)}) & (-p_{22}^{(1)}) \end{bmatrix} \begin{bmatrix} y_o \\ K^{-1}y'_o \end{bmatrix} + \begin{bmatrix} q_1^{(1)} \\ q_2^{(1)} \end{bmatrix} \right\} \tag{87}$$

For a general case where $m = 1,2,\ldots K-1$, we have by setting the coefficients of $\delta Y_3^{(m)}$ and $\delta Y_4^{(m)}$ in Eq. (83) to zero.

$$\begin{bmatrix} Y_3^{(m+1)} \\ Y_4^{(m+1)} \end{bmatrix} = \begin{bmatrix} p_{13}^{(m+1)} & p_{14}^{(m+1)} \\ p_{23}^{(m+1)} & p_{24}^{(m+1)} \end{bmatrix}^{-1}$$

$$\left\{ - \begin{bmatrix} (p_{11}^{(m+1)} + p_{33}^{(m)}) & (p_{12}^{(m+1)} + p34^{(m)}) \\ (p_{21}^{(m+1)} + p_{43}^{(m)}) & (p_{22}^{(m+1)} + p_{24}^{(m)}) \end{bmatrix} \begin{bmatrix} Y_3^{(m)} \\ Y_4^{(m)} \end{bmatrix} - \begin{bmatrix} p_{31}^{(m)} & p_{32}^{(m)} \\ p_{41}^{(m)} & p_{42}^{(m)} \end{bmatrix} \begin{bmatrix} Y_3^{(m-1)} \\ Y_4^{(m-1)} \end{bmatrix} + \begin{bmatrix} q_1^{(m+1)} + q_3^{(m)} \\ q_2^{(m+1)} + q_4^{(m)} \end{bmatrix} \right\} \tag{88}$$

We solve the above equation recursively for $Y_3^{(m+1)}$ and $Y_4^{(m+1)}$. Starting with $m = 1$ we have the initial conditions $Y_3^{(0)}$ and $Y_4^{(0)}$ and the solutions from Eq. (87) for $Y_3^{(1)}$ and $Y_4^{(1)}$. These values are substituted into Eq. (88) to obtain $Y_3^{(2)}$ and $Y_4^{(2)}$. From the values of $Y_3^{(1)}$, $Y_4^{(1)}$, $Y_3^{(2)}$, and $Y_4^{(2)}$ one can determine $Y_3^{(3)}$ and $Y_4^{(3)}$. This procedure continues until we obtain $Y3^{(K)}$ and $Y4^{(K)}$ which are the final values of the problem.

NUMERICAL RESULTS AND DISCUSSION

The analysis presented in previous sections will now be tested by way of some numerical examples. Let us consider a simple oscillator subjected to a harmonic force. The differential equation can be written as

$$m\ddot{y} + ky = f_o \cos \omega_f t \qquad 0 \leq t \leq T \tag{89a}$$

where T is some finite time of interest and a dot ($\dot{}$) denotes differentiation with respect to time. The initial conditions are

$$y(0) = y_o \quad \text{and} \quad \dot{y}(0) = y_o \tag{89b}$$

The system of Eqs. (89a) and (89b) is normalized with respect to T and it becomes

$$y^{*''} + k^* y^* = f^* \cos \omega_f^* t^* \qquad 0 \leq t^* \leq 1 \tag{90a}$$

and

$$y^*(0) = y_0^* \quad \text{and} \quad y^*(0) = y_0^* \tag{90b}$$

Through the following change of parameters

$$\begin{gathered}
t^* = \frac{t}{T} \quad , \quad dt^* = \frac{dt}{T} \\
y^*(t^*) = y(t) \quad , \quad y^{*'}(t^*) = T\frac{dy}{dt} \\
k^* = kT^2/m \quad , \quad f^* = f_o T^2/m \quad , \quad \omega_f^* = \omega_f T \\
y_0^* = y_0 \quad , \quad y_1^* = Ty_1
\end{gathered} \tag{91}$$

Comparing Eq. (90a) with Eqs. (24) and (1), one has

$$\begin{gathered}
\alpha = \text{constant} = 1 \quad , \quad \varepsilon = -1 \\
\beta = 0 \quad , \quad \gamma = 0 \quad \text{and} \quad Q = -f^* \cos \omega_f^* t^*
\end{gathered} \tag{92}$$

From the data presented here, we further set

$$m = 1.0 \quad , \quad k = 1.0 \quad , \quad t_0 = 1.0 \quad , \quad \omega_f = 0.5$$

The parameter T is given for each set of sample calculations.

First, Eq. (84) can be used exclusively to obtain all the solutions. This is demonstrated in Tables I through III. In these tables T has taken to be ten, five, and two, respectively and the number of steps for all cases is taken to be ten. Both y(t) and $\dot{y}(t)$ are shown and the exact solutions are given in parentheses for comparison. It is clear that the results are convergent, i.e., they are improved as the interval of time is decreased.

TABLE I. SOLUTION TO A FORCED VIBRATION PROBLEM OF A SIMPLE OSCILLATOR ($0 < t < 10$, Ten Steps. Exact Solution Shown in Parenthesis)

t	y(t)		$\dot{y}(t)$	
0	1.0000	(Given)	1.000	(Given)
2.0	1.7590	(1.7684)	-0.711	(-0.674)
4.0	-1.1495	(-1.0938)	-1.450	(-1.512)
6.0	-1.8534	(-1.9195)	0.867	(0.773)
8.0	0.2261	(0.1663)	0.564	(0.689)
10.0	-0.0531	(0.1139)	-0.404	(-0.381)

TABLE II. SOLUTIONS TO A FORCED VIBRATION PROBLEM OF A SIMPLE OSCILLATOR

($0 < t < 5$, Ten Steps. Exact Solutions Shown in Parentnesis)

t	y(t)		$\dot{y}(t)$	
0	1.0000	(Given)	1.0000	(Given)
1.0	1.8314	(1.8315)	0.4991	(.5012)
2.0	1.7646	(1.7684)	-0.6828	(-0.6740)
3.0	0.5536	(0.5654)	-1.6161	(-1.6079)
4.0	-1.1074	(-1.0938)	-1.5060	(-1.5121)
5.0	-2.1221	(-2.1217)	-0.4129	(-0.4350)

TABLE III. SOLUTIONS TO A FORCED VIBRATION PROBLEM OF A SIMPLE OSCILLATOR

($0 < t < 2.0$, Ten Steps. Exact Solutions Shown in Parenthesis)

t	y(t)		$\dot{y}(t)$	
0.0	1.0000	(Given)	1.0000	(Given)
0.4	1.3892	(1.3892)	0.9184	(.9184)
0.8	1.7132	(1.7132)	0.6760	(-0.6760)
1.2	1.9116	(1.9117)	0.2961	(0.2966)
1.6	1.9379	(1.9382)	-0.1752	(-0.1742)
2.0	1.7676	(1.7684)	-0.6754	(-0.6740)

Some discussion on the present formulation compared with previous work[3,4] is in order here. In previous work on unconstrained, adjoint variational formulation, the point of emphasis was to free the requirements of satisfying any of the initial conditions and to let the approximate solution converge to them. In the present analysis it is shown that the far end conditions need not be considered in a variational formulation of approximate solutions. A more detailed comparison in terms of numerical convergence, competency, efficiency, etc. is planned.

---

[3]J. J. Wu, "Solutions to Initial Value Problems By Use of Finite-Element-Unconstrained Variational Formulations," Journal of Sound and Vibration, 53, 1977, pp. 344-356.

[4]J. J. Wu and T. E. Simkins, "A Numerical Comparison Between Two Unconstrained Variational Formulations," Journal of Sound and Vibration, 72, 1980, pp. 491-506.

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